

ENERGY-BASED VARIATIONAL MODELING OF ADIABATIC SHEAR BANDS STRUCTURE

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Abstract. A modeling approach of the shear localization in thermoviscoplastic materials is developed in the framework of an energy-based variational formulation. The shear band structure in the layer (1D) sustaining a simple shearing deformation has been analysed in stationary and transient regimes. Starting from the optimization problem characterizing our variational formulation, we seek an approximate solution by way of a semi-analytical approach to predict the profiles of velocity and temperature in the band and obtain the evolution of some characteristic parameters, such as shear band width and maximum temperature, showing a good consistency with the solution obtained by the finite element method. Indeed, the results converge to the steady solution, in agreement with the canonical analytical solution [1].

1 INTRODUCTION

We have recently proposed a variational formulation of coupled thermo-mechanical boundary-value problems [2], allowing to write mechanical and thermal balance equations under the form of an optimization problem of a scalar function. This formulation applies to a wide range of material behaviors, possibly irreversible and dissipative, as long as they fit in the framework of Generalized Standard Materials [3]. The proposed variational structure brings several advantages. Beyond unifying a wide range of constitutive models in a common framework, the variational formulation also presents interesting mathematical properties. Among these, an important property is that of symmetry, inherent to all variational formulations, but which lacked to alternative coupled thermo-mechanical formulations previously proposed in the literature.

An adiabatic shear band is an intense shearing zone appearing in large plastic deformation with thermal instability at high strain rates. It's encountered in many engineering problems: forming processes and impact loading of metallic materials, but also in thermo-plastic polymers. Understanding and predicting their onset and evolution is critical since

they usually are a precursor to macroscopic ductile fracture. Much work has thus been published on the topic. Molinari ([1], [4]), Wright ([5]) have derived the analytical expressions for velocity and temperature profiles (1D) in the steady state, but the results are based on specific constitutive relations. In general, the small width of the shear band and the material softening effect associated with the local heating bring a lot of difficulties to numerical simulations, such as mesh dependence, model quality and interactions between multiple bands. Many methods (XFEM [6], meshless method [7], interface element [8], ...) have been used for bypassing these problems. However, it is necessary to know the approximate domain of the shear band width in most of these approaches. Here, we aim at constructing a semi-analytical model able to predict the internal structure of an adiabatic shear band and its evolution with time (and loading), starting from the variational formulation described in [2]. Indeed, thermo-mechanical coupling effects and conduction play a fundamental role in determining the velocity and temperature profiles within an adiabatic shear band.

2 Variational model in the steady state

We simplify the shear band model as its 1D problem illustrated in Fig.1: a layer of thickness $2H$ subjected to a simple shearing force. The velocity imposed on the boundary is V_0 , and isothermal conditions ($T = T_0$) at $y = \pm H$ are considered. The material is chosen as a steel having thermoviscoplastic properties with parameters of the material described in [1]. Here, the elastic and the hardening effects are neglected to simplify the model. First, we consider the problem in case of the steady state, when the stress and the entropy in the layer are stationary.

2.1 Variational formulation

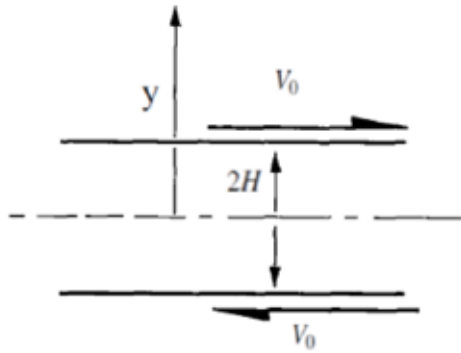


Figure 1: 1D shear band problem [1]

Using the total pseudo-potential function proposed by Yang et al.[2], and combined

with the stationary conditions, the power density function is reduced to :

$$\Phi(V, T) = \int_{-H}^H \Psi^*\left(\frac{T}{\Theta} V_{,y}; \Theta\right) - \chi\left(-\frac{T_{,y}}{T}; \Theta\right) dy$$

where Ψ^* is a dissipation pseudo-potential describing the viscoplasticity with thermal softening:

$$\Psi^*\left(\frac{T}{\Theta} V_{,y}; \Theta\right) = \frac{1}{m+1} \frac{\tau_0}{(\dot{\gamma}_0)^m} \exp\left[-\beta \left(\left(\frac{\Theta}{T_0}\right) - 1\right)\right] \left(V_{,y} \frac{T}{\Theta}\right)^{m+1} \quad m \in [0, 1] \quad (1)$$

Parameters m and β are the strain rate sensitivity exponent and the thermal softening coefficient, and τ_0 and $\dot{\gamma}_0$ are the reference stress and strain rate. $\Theta(y)$ is the equilibrium temperature introduced to satisfy the symmetry property of the power density function. χ is a thermal conduction pseudo-potential obeying the Fourier law:

$$\chi\left(-\frac{T_{,y}}{T}; \Theta\right) = \frac{1}{2} \lambda \Theta \left(\frac{T_{,y}}{T}\right)^2 \quad (2)$$

where the parameter λ is the thermal conductivity. Thus the problem of the shear band (Fig. 1) can be described as an optimization problem of the power density function:

$$\inf_V \max_T \{\Phi(V, T)\} \quad (3)$$

Taking variation with respect to the velocity, we can obtain the mechanical equilibrium equation, while the heat equation is obtained from stationarity condition on T . In addition, thermal equilibrium requires that $\Theta = T$.

2.2 Semi-analytical method

Considering boundary conditions in the 1D problem:

$$V|_{\pm H} = V_0; \quad T|_{\pm H} = T_0;$$

and taking advantage of the solutions obtained by Leroy and Molinari [1], the profiles of velocity and temperature can be written as follows with parameters h and T_{max} :

$$V(y) = V_0 \frac{\tanh(y/h)}{\tanh(H/h)}, \quad T(y) = T_{max} - (T_{max} - T_0) \frac{\ln(\cosh(y/h))}{\ln(\cosh(H/h))} \quad (4)$$

where h is the shear band width, and T_{max} is the central temperature. We introduce a new parameter T_{max} to replace the material parameters used in [1], since this change avoids the limitation to specific constitutive relations and gives us a more general description of velocity and temperature in the layer.

Finally, the variational model of the shear band in the steady state is restated as follows:

$$\inf_h \max_{T_{max}} \{\Phi(h, T_{max})\} \quad (5)$$

2.3 Results

In our calculations, a trust region method is used in view of the strong non-linearity of the Euler-Lagrange equations of (5). Table (1) shows the shear band widths and the central temperatures for different material parameters, in good agreement with the analytical solutions.

Table 1: Shear band width and central temperature (dimensionless) ($\beta = 0.38$; $V_0 = 0.1108$ m/s)

	variational model $[h \ T_{max}]$		analytical $[h \ T_{max}]$	
$m = 0.12; \kappa = 1/0.242373$	0.312643	775.026	0.312643	775.020
$m = 0.012; \kappa = 1/0.403788$	0.031073	896.626	0.031072	896.656
$m = 0.06; \kappa = 1/0.3218$	0.153552	851.299	0.153552	851.303

Fig. 2 illustrates the influence of the imposed velocity V_0 on h and T_{max} . With the velocity increased, the shear band width h decreases and the central temperature in the band increases. Obviously in a thermal softening material, a higher strain rate causes a smaller band width, and also brings more dissipation and heat generation in the band. In addition, the time of the formation of the shear band is so short that the heat cannot go out of the layer by conduction, leading to a higher central temperature.

3 Variational model in transient regime

For thermoviscoplastic materials under high strain rates, the rapid evolution of the shear band and its small width complicate numerical simulations. In this section, we will extend the stationary variational modeling to transient regime, establishing a variational update form of the 1D shear band problem.

3.1 Incremental variational formulation

The variational framework proposed in Yang et al.[2] also includes a time-discretized incremental variational problem, and it can be applied to the 1D shear band problem, yielding an incremental optimization problem. In particular, considering a time increment $[t_n, t_{n+1}]$, and assuming that $[\mathbf{F}_n, T_n, \mathbf{F}_n^p]$ is known, we proceed to obtain the variational update at time t_{n+1} . \mathbf{F} is the gradient of deformation, and we consider the conventional multiplicative decomposition:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$$

If the material satisfy the Von Mises law, the gradient of plastic deformation \mathbf{F}_{n+1}^p verifies the following equalities:

$$\mathbf{F}_{n+1}^p = \exp[(\bar{\varepsilon}_{n+1}^p - \bar{\varepsilon}_n^p) \mathbf{M}] \mathbf{F}_n^p$$

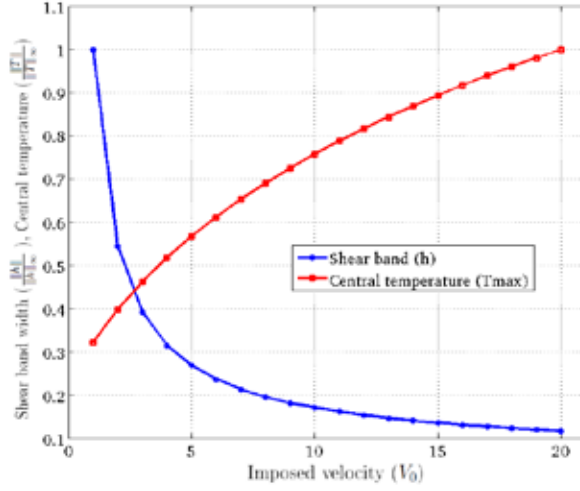


Figure 2: Influence of the imposed velocity V_0 about the shear band width and the central temperature

$$tr(\mathbf{M}) = 0, \quad \mathbf{M} \cdot \mathbf{M} = \frac{3}{2}$$

where $\bar{\varepsilon}^p$ is the cumulated plastic deformation. In general, \mathbf{F} is written:

$$\mathbf{F}_{n+1} = \mathbf{I} + \frac{\partial \overrightarrow{u_{n+1}}}{\partial \overrightarrow{x}}$$

Considering the 1D shear band problem, it reduces to:

$$\mathbf{F}_{n+1} = \begin{bmatrix} 1 & \frac{\partial u_{n+1}}{\partial y} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Following [2], the total pseudo-potential for the thermo-mechanical coupled problem is then:

$$\Phi_n = \int_{-H}^H \left[\mathcal{W}_n - \Delta t \chi \left(\frac{1}{T_{n+1}} \frac{\partial T_{n+1}}{\partial y} \right) \right] dy$$

where \mathcal{W}_n is the optimized potential about $\bar{\varepsilon}_{n+1}^p$ and \mathbf{M} :

$$\begin{aligned} \mathcal{W}_n(\mathbf{F}_{n+1}, T_{n+1}; \mathbf{F}_n, T_n, \mathbf{F}_n^p, \bar{\varepsilon}_n^p) &= \inf_{\bar{\varepsilon}_{n+1}^p, \mathbf{M}} [W(\mathbf{F}_{n+1}, T_{n+1}, \mathbf{F}_{n+1}^p, \bar{\varepsilon}_{n+1}^p) \\ &\quad - W(\mathbf{F}_n, T_n, \mathbf{F}_n^p, \bar{\varepsilon}_n^p) + \eta_n (T_{n+1} - T_n) \\ &\quad + \int_{t_n}^{t_{n+1}} \Psi^* \left(\frac{T_{n+1}}{T_n} \frac{\Delta \bar{\varepsilon}^p}{\Delta t}; T(t) \right) dt] \end{aligned} \quad (6)$$

where $W(\mathbf{F}_{n+1}, T_{n+1}, \mathbf{F}_{n+1}^p, \bar{\varepsilon}_{n+1}^p)$ is the free energy, which includes the elastic energy, stored plastic energy and the heat storage capacity of the material [9]. In addition, the

notations Ψ^* and χ are the same as previously: the dissipation pseudo-potential and the Fourier pseudo-potential. The entropy η_n is defined by :

$$\eta_n = -W_{,T_n}(\mathbf{F}_n, T_n, \mathbf{F}_n^p, \bar{\epsilon}_n^p)$$

and $\Delta\bar{\epsilon}^p = \bar{\epsilon}_{n+1}^p - \bar{\epsilon}_n^p$. Note that \mathcal{W} appears as a thermo-elastic pseudo-potential. Indeed Piola-Kirchhoff stress can be written as:

$$\frac{\partial \mathcal{W}_n}{\partial \mathbf{F}_{n+1}} = \mathbf{P}_{n+1}$$

and the heat equation in the adiabatic form is given by taking variation about T :

$$\frac{\partial \mathcal{W}_n}{\partial T_{n+1}} = -\Delta\eta + \frac{\Delta t}{T_{n+1}} D_{int}$$

where D_{int} is the internal dissipation.

In view of the above variational framework, the incremental 1D problem of the shear band described in Fig.1 is written as:

$$\inf_{u_{n+1}} \max_{T_{n+1}} \Phi_n(u_{n+1}, T_{n+1}; u_n, T_n, \mathbf{F}_n^p, \bar{\epsilon}_n^p) \quad (7)$$

When the time step tends towards 0, Euler-Lagrange equations of (7) are consistent with continuous mechanical and thermal equilibrium equations.

3.2 Numerical validation

In this section, we will use the finite element method (FEM) and a semi-analytical method to simulate the evolution of velocity and temperature in the layer. On the one hand, FEM gives us a more precise simulation of the formation of the shear band. However, it cannot avoid the difficulty of mesh dependence, the domain where the shear band occurs requiring a very fine mesh; on the other hand, the semi-analytical method, although less precise in early stages of shear band formation, shows a good convergence of the shear band width and is consistent with the results obtained by FEM. In addition, it has a better efficiency compared with FEM.

3.2.1 Finite element method

Thanks to the symmetry of the total pseudo-potential, the tangent matrix of the FEM is also symmetrical, which is different from the traditional thermal-mechanical problem, and this character brings some algorithmic advantages. In the FEM model, elasticity and thermal capacity are considered [9]. But hardening effect is neglected for comparing with analytical results. Because of the thermal softening in the dissipation pseudo-potential, we choose the following form for its time-discretization [10]:

$$\frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \Psi^* \left(\frac{T_{n+1}}{T_n} \frac{\Delta \bar{\epsilon}^p}{\Delta t}; T(t) \right) dt \approx \frac{T_n}{T_{n+1}} \Psi^* \left(\frac{T_{n+1}}{T_n} \frac{\Delta \bar{\epsilon}^p}{\Delta t}; T_n \right) + \frac{\Delta T}{T_{n+1}} \Psi^* \left(\frac{T_{n+1}}{T_n} \frac{\Delta \bar{\epsilon}^p}{\Delta t}; T_{n+\alpha} \right)$$

The parameter α is chosen equal to 0.5. In the latter simulation by the semi-analytical method, we also use this form to approximate the dissipation, but α is chosen equal to 0.

Fig.3 gives us the results for profiles of velocity and temperature in the layer ($H = 1.25\text{mm}$, $V_0 = 0.01108\text{m/s}$, $T_0 = 300\text{K}$). As time increases, profiles of velocity change from a linear form to a nonlinear form, and step by step concentrate in the central zone, arriving at a steady state when time reaches 0.1 s. The stationary shear band width is 0.247 mm , and $T_{max} = 395\text{K}$.

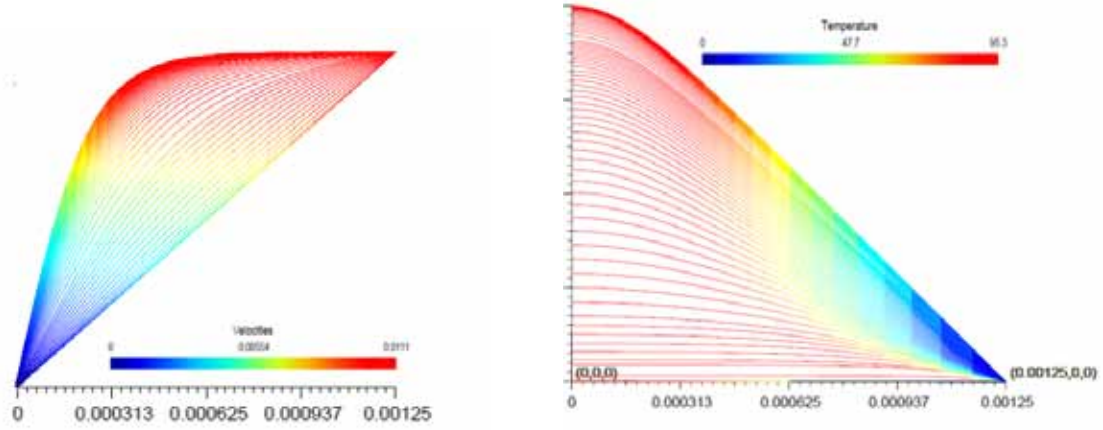


Figure 3: Evolution of the profiles of velocity and temperature ($V_0 = 0.01108\text{m/s}$)

We also analyse the evolution of the shear band when the imposed velocity is 1m/s (Fig.4). Compared with $V_0 = 0.01108\text{m/s}$, the time when the material reaches a steady state is shorter, the shear band width is smaller ($h = 0.014583\text{mm}$), and the central temperature is higher ($T_{max} = 2047\text{K}$), which is in agreement with the analytical solution. In addition, we can observe a heat affected zone in the process of the formation of the shear band because of the locally lower strain and the local annealing due to the temperature increase [4]. This transient effect is less obvious in the case of $V_0 = 0.01108\text{m/s}$.

For illustrating the evolution of shear band width and comparing it with the semi-analytical method, we choose two parameters to measure the shear localization: the kinematic width h_v from the velocity distribution and the thermal width h_T from the temperature distribution. Referring to the analytical formulation, they are calculated by:

$$\begin{aligned} h_{V_{n+1}} & \quad \text{such that} \quad V_{n+1}(h_{V_{n+1}}) \simeq V_0 \tanh(1) \\ h_{T_{n+1}} & \quad \text{such that} \quad \frac{2m}{\beta} \log(\cosh(\frac{H}{h_{T_{n+1}}})) = \frac{T_{max}}{T_0} - 1 \end{aligned}$$

Fig.5 presents the convergence of the kinematic width and the thermal width when $H = 1.25\text{mm}$, $V_0 = 0.01108\text{m/s}$, $T_0 = 300\text{K}$. With the time increased, the two widths decrease

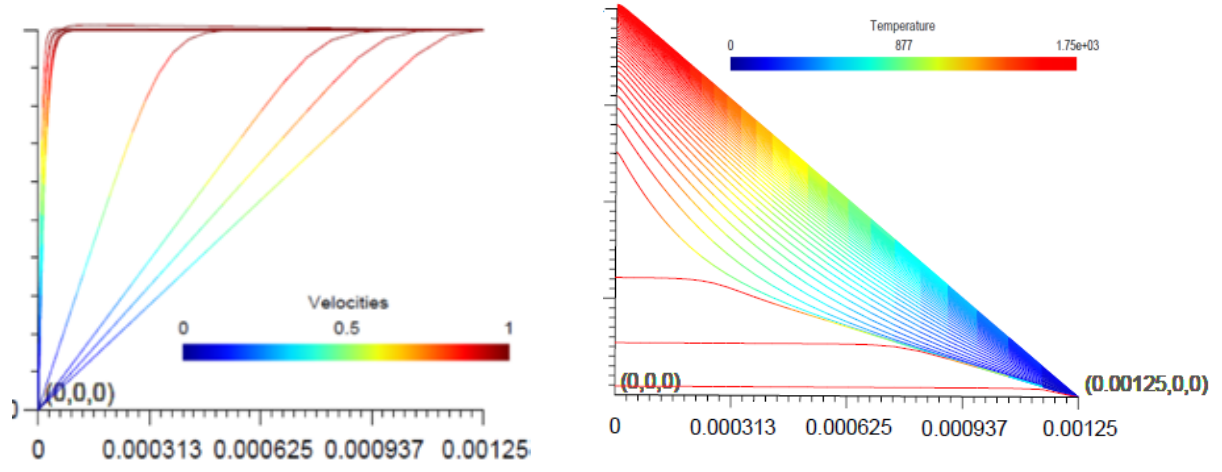


Figure 4: Evolution of the profiles of velocity and temperature ($V_0 = 1m/s$)

gradually and tends towards the same stationary value, which is consistent with the analytical solution.

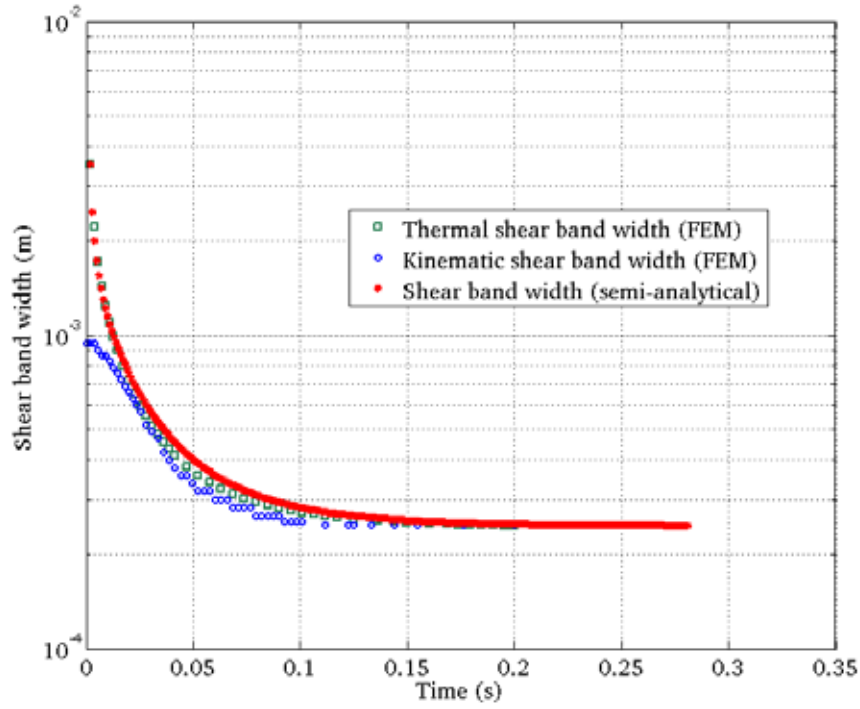


Figure 5: Convergence of the shear band width ($V_0 = 0.01108m/s$)

3.2.2 Semi-analytical method

The strong shear localization causes difficulties in the simulation of the shear band by FEM. Indeed, it is necessary to have an approximation of the width before constructing the mesh. Therefore, we follow an idea initially proposed by Yang et al.[8], who derived a simple model of shear bands based on a linear velocity and a Gaussian temperature profiles. Neglecting the heat affected zone, and supposing that at each time step the distributions of velocity and temperature satisfy the canonical solutions, we write at $t = t_{n+1}$:

$$V(y) = V_0 \frac{\tanh(y/h_{n+1})}{\tanh(H/h_{n+1})}, \quad T(y) = T_0 - \frac{2m}{\beta} T_0 \ln \frac{\cosh(y/h_{n+1})}{\cosh(H/h_{n+1})} \quad (8)$$

where m, β are the material parameters, the same as the analysis in the steady state. We then obtain the incremental optimization problem for the 1D shear band (Fig.1) as:

$$\text{stat}_{h_{n+1}} \Phi_n(h_{n+1}) \quad (9)$$

It is important to note that, in contrast to previous approaches, the shear band width figures among the unknowns, and will be determined by computation. It is an important feature, since this width is controlled by the combined effect of internal dissipation and conduction, and we will use an example to illustrate that it can evolve as the shear band evolves towards its stationary structure.

In general, there is no shear band in the plane at the initial time, so we choose:

$$h_0 = H$$

Fig.6 shows us the evolution of velocity profiles and temperature profiles compared with the analytical stationary solutions when $H = 1.25\text{mm}$, $V_0 = 0.01108\text{m/s}$, $T_0 = 300\text{K}$. Here the time step is chosen as $\Delta t = 1e - 3\text{s}$. Results obtained by the semi-analytical approach are consistent with those obtained by FEM. In addition, returning to Fig.5, we can get the comparison about the convergence of shear band width. The widths evolutions are in agreement with the results by FEM. Furthermore, computation time is reduced compared to that of FEM. Therefore the semi-analytical method presents a higher efficiency besides not requiring a mesh.

4 CONCLUSIONS

Considering a simplified 1D model of shear band in thermoviscoplastic materials, we have developped an energy-based variational semi-analytical approach to predict shear band internal structure. In stationary or transient regimes, the shear band width and the central temperature are determined and in good agreement with the work of Leroy et al.[1]. Compared with the finite element method, we not only got the validation of the variational modeling in the analysis of the formation of the shear band, but have also shown the efficiency and feasibility of the proposed semi-analytical method.

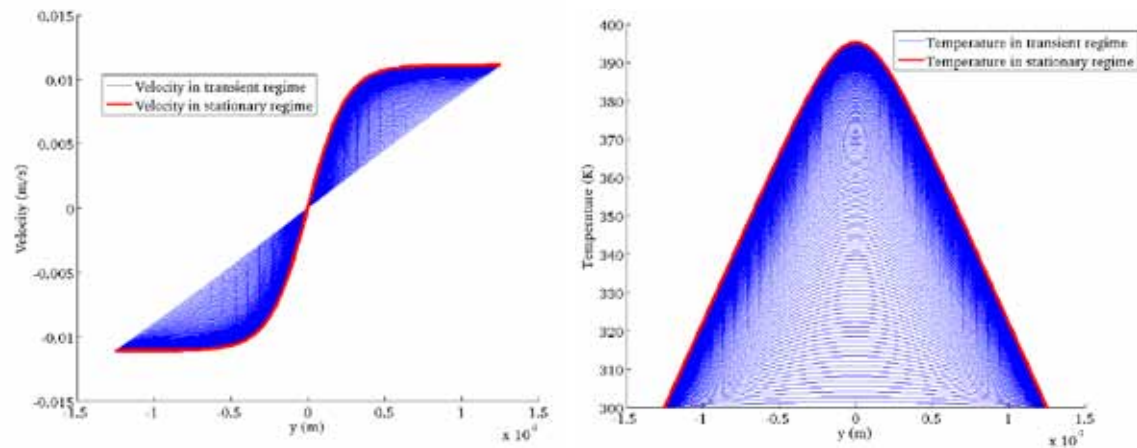


Figure 6: Evolution of the profiles of velocity and temperature by semi-analytical method ($V_0 = 0.01108\text{m/s}$)

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